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In this paper we analyse the results of one of the most comprehensive models of ocean biogeochemistry with an emphasis on biogeographic validation sensu Longhurst (Ecological Geography of the Sea, 2007, 2nd edition, Academic Press). A set of multivariate statistical tools, Multi Dimensional Scaling (MDS) and Principal Components Analysis (PCA), are used to verify the existence of pre-defined biogeographic provinces and their statistical significance. The MDS ordination indicates that the given provinces are recognizable in the model on the basis of the selected variables. Analysis of Similarity (ANOSIM) shows that the provinces are statistically separable and they can be more easily distinguished in terms of their environmental features rather than their biology. The underlying relationships between the physical and

biological properties are investigated through correlation analyses, thus providing some insights on how the model reproduces features characteristic of the various regions.

Satellite chlorophyll data have been used to demonstrate external validation at the biogeographic level. The a priori provinces as characterised by chlorophyll values cannot be statistically separated in either the data or the model. It is likely this is related to the arbitrary choice of province boundaries, which are not necessarily the same as those derivable from non-interpolated SeaWiFS data.

The PCA comparison of modelled and observed chlorophyll demonstrated some objective skill in the model as it generally captures the dominant mode of the data, although severe mismatch was identified in certain regions by visual comparison (Indian and Southern Oceans). The model also overestimated seasonal variability compared to the data. The method shows promise for helping overcome problems with model verification due to undersampling of most ocean biogeochemical variables.

Biogeographic validation of a global ocean biogeochemical model

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Abstract

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1 Introduction

There have been several attempts at providing a conceptual classification of the pelagic marine environment, based mainly on either the biogeography of distinct taxonomic groups (e.g. copepods) or the spatial variability of physical properties, such as temperature, salinity and turbulence (reviewed by Longhurst, 2007). The advent of ocean colour remote sensing stimulated attempts to address this limitation and was used as the basis for a series of classifications based on empirically-derived chlorophyll and primary production estimates (Longhurst, 1995; Longhurst et al., 1995; Sathyendranath et al., 1995). Longhurst's (2007) partition of the oceans into four major biomes, based on observed or inferred physical processes affecting stability and mixing in the upper ocean (polar, westerlies, trade winds, tropical), realised as ~50 ocean provinces (regional expressions of different biomes), remains the most widely-accepted ocean classification to date and has been of much use as a framework in the estimation of oceanic primary production and biogeochemical budgets.

The concept of provinces is based on the observation that large ocean regions are characterised by coherent biological conditions and physical forcing, and that these regions are representative of macro-scale ocean ecosystems (Longhurst, 2007; Hardman-Mountford et al., accepted). However, as also pointed out by Longhurst, the boundaries between provinces are substantially ephemeral, because they are linked to physical properties which are known to change seasonally and inter-annually. Longhurst (2007) additionally suggests that the boundaries which were selected subjectively and intuitively on the basis of climatological data be further identified by i) comparing the distribution of individual biota between provinces, ii) testing statistically different conditions in adjacent provinces, or iii) using analytical techniques to partition a relevant global data set. Hardman-Mountford et al. (accepted) have applied a range of multivariate statistics to a satellite-derived chlorophyll

climatology to provide an objective classification of the ocean into several macro-scale biomes associated with trophic status (eutrophic, mesotrophic, oligotrophic). The regional realisations of these biomes constitute provinces and have properties consistent with ecological systems. Recently, Gregr and Bodtker (2007), have applied adaptive classification algorithms to selected physical variables from a general circulation model output in order to partition the northern Pacific into significant distinct regions. They identified contiguous oceanic regions which could be related to well-known water-masses, also finding significant correspondence with the spatial distribution of satellite chlorophyll.

Ocean Biogeochemistry General Circulation Models (OBGCM) are indeed suitable tools to perform statistical and/or analytical tests on the significance of biomes and provinces. There are several cases of OBGCMs which are capable of visually reproducing the major spatial features of global ocean biogeochemistry (e.g. oligotrophic gyres, upwelling regions), ranging from those with simple implicit representations of biology to others which explicitly realize several dynamic plankton functional types (Six and Meier-Reimer, 1996; Aumont et al., 2001; Gregg et al., 2003; Moore et al., 2004; Le Quéré et al., 2005; Vichi et al., 2007b, among others). Notwithstanding the different degrees of complexity of the various approaches, most of these models show a visual separation in biogeochemical regions which roughly correspond to the chlorophyll distribution observed from space. This kind of comparison (face validity) is done at the level of a bulk property of the marine ecosystem and tells us very little about the intrinsic capability of the model to simulate the biogeochemical features of each single region. Further visual comparisons involving satellite-derived Phytoplankton Functional Type (PFT) distributions at the global scale have been attempted (Vichi et al., 2007b, using data from Alvain et al., 2005), though a direct comparison with relevant ecosystem properties is probably still lacking (Anderson, 2005).

Historically there has been a lack of objective, quantitative comparison between biogeochemistry model results and observation data in OBGCMs. This can partly be attributed to a lack of data (or ease of access to global data) and partly to a cultural acceptance that a subjective visual comparison, especially with global ocean models, is acceptable. This behaviour is still widespread despite the precautionary warnings that have been raised in the ecological modelling community since the seminal paper of Ryckiel (1996). A systematic analysis of the performance of 153 biological models that include plankton demonstrated that the efforts over the last decade to increase the level of biological detail and spatial complexity have not led to a systematic or demonstrable improvement in model performance (Arhonditsis and Brett, 2004; Arhonditsis et al., 2006).

It is therefore necessary to move beyond face validity, and to analyse whether and where these models have skill in order to determine their real theoretical validity. By taking subjective, qualitative validity as a starting point, it is suggested to move through objective qualitative validity towards quantitative validation. Our approach involves the application of multivariate statistical analyses to global ocean model outputs, building on the experience obtained in a regional ocean model application of this method (Allen et al., 2007).

This work is a first step towards this approach, stemming from the widely-held premise that biogeochemical provinces correspond to real ecological structure (supported at the biome level by the objective analyses of Hardman-Mountford et al., accepted). By taking a likely set of predefined provinces (the Longhurst provinces), we aim to verify whether they qualitatively exist in the model and have distinct credible physical and biological properties. The basic questions are (1) Can we identify Longhurst provinces in the model? (2) Are the provinces in the model statistically separable and related to identifiable physical conditions? (3) Are the modelled provinces emergent biogeochemical features of the model, which derive from the dynamical interaction of physical and biological processes?

For the purpose of this study, Longhurst provinces are taken as useful reference structures. Although their exact spatial extent and distribution has not been objectively confirmed, as occurs for terrestrial biogeography, they can still be usefully applied as hypothetical regions related to ocean dynamics. The study could therefore be repeated with a different choice of provinces, so our major aim is not to question the regions themselves, but rather to apply them as a useful concept for model validation. If these regions are physically coherent and statistically separable in both model output and data, it becomes possible to undertake validation. In the second part of the work we present a first example of this validation approach with satellite chlorophyll data from SeaWiFS by means of multivariate statistical tools.

2 Methods

2.1 Biogeochemical model

The global ocean biogeochemical model in this study is PELAGOS (PELAgic biogeochemistry for Global Ocean Simulations, Vichi et al., 2007a,b), which is a coupling between the OPA (Océan PArallélisé) general circulation model (Madec et al., 1999) and the global ocean version of the Biogeochemical Flux Model (BFM, http://bfm.cmcc.it) derived and modified from the ERSEM model (Baretta et al., 1995). The model grid is the irregular ORCA2 configuration (Madec and Imbard, 1996) with a nominal 2 x 2 degrees size and a refined latitudinal mesh of 0.5 degree in the equatorial and Southern Ocean regions.

The biogeochemical model implements a set of biomass-based differential equations that solves the fluxes of carbon, nitrogen, phosphorus, silica and iron among selected biological functional groups representing the major components of the lower trophic levels. The PFTs in the pelagic environment are represented by unicellular planktonic autotrophs

(pico-, nano-phytoplankton and diatoms), zooplankton (nano-, micro- and meso-) and heterotrophic bacterio- plankton. The model also simulates the dynamics of nitrate, ammonium, phosphate, biogenic silicate, iron, oxygen and has an explicit parameterization of the biochemical cycling of dissolved/particulate non-living organic matter.

The climatological features of the model have been analysed in a perpetual year context in Vichi et al., (2007b). The results analysed here are extracted from an inter-annual simulation over the period 1958-2001 forced with daily mean heat and momentum fluxes from the European Centre for Medium Range Weather Forecasting (ECMWF) 40-year re-analysis (ERA-40, Uppala et al., 2005). In this paper we focus on the period of the simulation when satellite ocean colour data from the Sea-viewing Wide Field-of-view Sensor (SeaWiFS) are also available (1998-2001). Sea surface temperature (SST) is relaxed to the daily-interpolated value of the Reynolds data set (Reynolds et al., 2002). Other ocean physics parameterizations are as in Vichi et al. (2007b).

The major differences with the climatological simulations are due to a trial and error manual re-calibration of some of the parameters, namely nutrient availability for all PFTs and the iron limitation threshold for diatoms. The BFM website provides a link to a new table of parameters to be compared with the one in Vichi et al. (2007b).

2.2 Satellite ocean colour data

Monthly composites of global satellite Chlorophyll-a level 3 products, derived from visible spectral radiometer (ocean colour) data from SeaWiFS on board the OrbView-2 satellite, were obtained from the US National Aeronautics and Space Administration (NASA). The composites were spatially interpolated and averaged over the time period Jan 1998 – Dec 2001 to produce climatological means for each month that match the model spatial and temporal resolution. The latitudinal extent of data retrieval by SeaWiFS is limited for the winter season in each hemisphere. For spatial Principal Components Analysis (PCA), the

same spatial extent must be used for each variable (time step), so only data between 50°N and 50°S were used for each month in these analyses.

2.3 Multivariate statistical analyses

Non-metric multi-dimensional scaling ordination (MDS) was used to visualise in a 2-dimensional space the proximities between provinces according to the extracted multivariate set of variables. MDS is a powerful statistical tool that creates a spatial ordination of the data which carefully maintains the similarities or dissimilarities between the objects. In our case, the objects are the provinces, characterised by a multivariate combination of means and variances of the major biogeochemical properties (see Sec. 2.5). Due to the kind of the data set, which contains both physical and biological information, the resemblance matrices carrying the proximity information between provinces are obtained from normalised Euclidean distances.

Groups of similar provinces were identified by hierarchical group-average clustering. Once the dendrogram was complete, groups were separated with two different methods: 1) by taking a slice at an arbitrary distance in the dendrogram, and 2) by applying the SIMPROF analysis (Clarke and Gorley, 2006). The latter tests the significance of each split in the dendrogram by means of a statistic applied to a sample of the possible permutations of the variable values involved in that split. The null hypothesis is that there is no structure in the cluster configuration. The results of both groupings are also shown in the MDS space.

Differences between province pairs were tested for statistical significance using analysis of similarities (ANOSIM, Clarke and Green, 1988). The ANOSIM statistic (R) compares the similarity of ranked variables within a province with the average rank of different provinces and it is scaled to vary between −1 and +1. A value of +1 indicates that the similarity between all samples within one province is higher than all similarities between groups.

Principal component analysis (PCA), also known as Empirical Orthogonal Function (EOF) analysis in meteorology and oceanography (Preisendorfer, 1988), is a commonly used multivariate statistical technique related to factor analysis, which attempts to disentangle complicated inter-relationships in high-dimensionality data sets by reducing the number of significant variables and transforming them to independence (Kendall and Stuart, 1966). It works upon the variance structure of the data to determine its dimensions upon linearly uncorrelated, or orthogonal, axes. PCA has the characteristics of preserving the total variance in the transformation and minimising the mean square approximate errors (Fung and LeDrew 1987). In this study, PCA was performed in two different configurations: 1) variables are three statistical properties of modelled or observed chlorophyll fields (mean, spatial and temporal standard deviation) and samples are spatial locations; 2) variables are time steps of modelled or observed chlorophyll fields and samples are spatial locations.

Numerical computations and visualisations were performed with PRIMER v 6 (Clarke and Warwick, 2001; Clarke and Gorley, 2006), MATLAB and ERDAS Imagine v 8.7 (Leica, 2003). The ANOSIM MATLAB implementation is provided by Jones (2002).

2.4 Longhurst provinces in the model domain

The name and definition of provinces are derived from Longhurst (1998), according to the spreadsheet available at http://www.mar.dfo-mpo.gc.ca/science/ocean/BedfordBasin/Papers/Longhurst1998/Provinces/EcologicalGeographyOfTheSea.htm. Longhurst's provinces have been mapped on the model grid as shown in Figure 1 by taking into account known model features and biases (e.g. Doney et al., 2004). The resolution of the model has indeed limited skill in capturing the physical dynamics of coastal biomes, and therefore most of the related provinces have been joined to the adjacent more open-ocean regions. However some coastal provinces have been retained (e.g. the

Mauritanian-Moroccan upwelling, CNRY, and the NE Atlantic Shelves) as examples to test the performance of the model. The localisation of major physical boundaries, such as the extent of the Pacific Equatorial Divergence (PEQD) into the Western Pacific Warm Pool (WARM), was determined subjectively from the mean annual position of the physical features.

2.5 Model sampling strategy

The analysed model variables were divided in 2 major groups: environmental and biological. Environmental variables are considered to be the physical and hydro-chemical indicators of the state of the water masses. They are both surface variables as sea surface temperature (SST), short wave radiation (SWR), salinity (SAL) and measures of upper ocean dynamics, such as mixed layer (MLD) and thermocline (TCD) depths. Hydrochemistry is represented by the surface concentrations of modelled nutrients: phosphate (N1), nitrate (N3), ammonia (N4), silicate (N5) and iron (N7). These variables are actually modified both by hydrodynamics and by the uptake and remineralisation of plankton functional groups.

The biological variables are the surface concentrations of chlorophyll and carbon content of phytoplankton (diatoms = P1, flagellates = P2, picophytoplankton = P3), and the carbon biomass of heterotrophs (bacteria = B, microzooplankton = Z5, heterotrophic nanoflagellates = Z6 and omnivorous mesozooplankton = Z4). Total chlorophyll was only considered when comparing with SeaWiFS data. The target temporal window is the seasonal scale and monthly means of the relevant variables over the 4-year period 1998-2001.

Different strategies have been used to extract model properties from the given set of provinces. Bulk sampling refers to the computation of mean values and standard deviations as measures of the model variability within each province (spatial variability of the annual mean over the province and temporal variability of the spatial mean over the year). Area-weighted sampling implies that the number of extracted samples is proportional to the surface of the

province, with a minimum of 2 samples from the smallest province. The largest one, i.e. the Southern Pacific Subtropical Gyre (SPSG, province 59), has 136 randomly distributed samples.

As a final strategy, we considered a purely random sampling, where a fixed number of samples is extracted from the dataset. Not all the provinces will be represented with this method as it is likely that largest regions (or regions with larger number of grid points in the ORCA2 grid, as the equatorial ones) will have more samples.

3 Model validation

3.1 Visual comparison

Figure 2 shows a comparison of model chlorophyll and SeaWiFS data to demonstrate the first stage of face validity, the same as done in Vichi et al., (2007b) for the climatological simulations. Model chlorophyll was computed by summing together the chlorophyll content of all phytoplankton groups integrated over one optical depth to be comparable to satellite observations (Vichi et al., 2007b). The overall result is a better representation of the northern hemisphere high latitudes and of the equatorial Pacific divergence in comparison with Vichi et al. (2007b), although chlorophyll is now slightly overestimated in the latter. Apart from the lack of coastal maxima, the largest biases are clearly in the Southern Ocean and in the Indian Ocean, with an overestimation in the former and a marked absence of phytoplankton in the whole northern Indian Ocean.

Figure 3 shows an example of the seasonal cycle of chlorophyll in the North Atlantic Drift Region (NADR) and in the Pacific Equatorial Divergence (PEQD), as presented in a climatological context by Vichi et al. (2007b). The model has improved with respect to the climatological results, particularly during the North Atlantic spring; this is mostly due to the

relaxation of iron limitation on diatom growth, which however partly contributed to the overestimation in the Southern Ocean.

While further speculative inferences could be drawn from this kind of visual inspection, nothing can be said other than the model produces a reasonable spatial structure and that the seasonal variability is within the range of observations. Face validity is a first necessary step, yet its interpretation is purely subjective and strongly based on the choice of colours, axes intervals or contour levels.

Additional information can indeed be provided with spatial maps of differences between model and data. These representations, though being a stricter point-to-point comparison, are still regarded as face validity because patterns are generally interpreted visually. Moreover, this kind of analysis would highlight the largest biases and possibly mask other important features, thus the interpretation of these information would still be strongly based on subjectivity.

3.2 Does the model have a distinct biogeography?

In order to assess whether or not the model has a distinct biogeography, we use MDS to visualise in 2 dimensions the multivariate bulk properties (see. Sec. 2.5) of each Longhurst province. The MDS ordination obtained from the full data set of bulk properties of each region is shown in Figure 4. The stress value of the MDS is 0.12, which is close to a good representation of the underlying relationships. The groups obtained from the hierarchical cluster analysis at 2 arbitrary distances and the results of the SIMPROF analysis are superimposed to the MDS with ellipses and symbols, respectively.

Figure 4 shows two major clusters of regions and one single province (the GIN (Greenland, Iceland and Norwegian) seas, SARC) representing the polar biomes, and a large group corresponding to the mid-latitude and inter-tropical provinces. The SIMPROF analysis however indicates that more provinces can be distinctively separated from the others on the

basis of their bulk properties and statistical features. Among them, we find the Bering Sea, the north-western shelf of the North Atlantic and the Pacific Equatorial Divergence (PEQD). The Antarctic polar biome is clearly separated but clustered together with the sub-Arctic and sub-Antarctic provinces. It is indeed likely to interpret this as a similarity between sub-polar regions above (below) 50° N (S) in the model. The provinces belonging to the Southern Ocean polar front (provinces 21 and 80) are clearly identifiable as dynamical regions with distinctive features with respect to the others, but not between each other as revealed by the SIMPROF.

A similar consideration can be made for the provinces 10, 31, 32 and 64 which belong to the same latitudinal band in the southern parts of the Indian and Atlantic oceans (Figure 1). They are very close to the northern subtropical Atlantic in the MDS representation (provinces 6 and 18) indicating that the intuitively similar oceanographic features determine largely their behaviour in the model.

The subtropical gyre provinces are clustered separately from the inter-tropical and equatorial regions, with the NE Pacific set in the middle. Much more distinguishable are the Kuroshio province and the enclosed seas (Mediterranean and Red Sea).

The environmental variables are also representable in the MDS space (Figure 5) with a smaller stress value of 0.1, indicating a good level of scaling in reduced space. Environmentally, the Antarctic is very separate, as it was also observed in Figure 4 where all the variables were considered. On the other hand, the PEQD (province 62) is clustered together with the tropical and sub-tropical seas indicating similar environmental properties, while it is clearly separated in the full-set MDS (Figure 4). Province 12, the North African upwelling, is thus not distinguishable, in terms of mean and variability, from the other Atlantic regions of the tropical band. This confirms that the physical model is not able to develop distinctive coastal features.

The North Atlantic regions (2, 3, 4 and 5) are relatively distant from each other and were separated in the MDS representation obtained from the full set of variables (Figure 4). However, the SIMPROF analysis gives indications that from an environmental point of view, they do correspond to the same larger-scale biome, and that the biology separates it in smaller distinct provinces.

The MDS of the biological variables (Figure 6) shows lesser separation between provinces with respect to the environmental variables. The exceptions are the GIN seas, the Southern Ocean Polar Front (21 and 80) and the PEQD (province 62). This MDS representation explains the contrasting position of the PEQD between Figure 4 and Figure 5. This province is characterised by distinct biological properties which increase the dissimilarity in the full data set despite the resemblance of the environmental features. Similar considerations are valid for the GIN seas and the Falkland, which are distinguished in the analysis of the full set of variables because of their biological features (Figure 4).

Two major groups of provinces are identified which we may classify more as a functional biome ordination than a geographical separation. The cluster analysis groups all the sub-polar frontal regions separately from the sub- and inter-tropical provinces. In addition, the SIMPROF test gives a statistically significant split between the sub-polar seas of the Atlantic and Southern Ocean and the North Pacific, which are quite well separated from the North Atlantic Gulf Stream and NADR provinces. The corresponding eastern boundary current in the Pacific Ocean (53 and 54) is instead close to the other subtropical provinces and not characterised by distinctive biological features.

The other inter-tropical Pacific and Atlantic regions are not clearly separable from a biological point of view as they were in the environmental MDS. This may be interpreted as a limited capability of the model in capturing either the physical and/or biological features which have led to the classification of these provinces as biogeographically distinct.

3.3 Significance of the provinces

This section investigates the statistical separation between the provinces by comparing samples extracted from the model output. Both the area-weighted and random sampling described in Sec. 2.4 were used to characterise each province. The results from the ANOSIM test are listed in Table 1 where the global R statistic (Clarke and Green, 1988) is reported for all the variables and for the environmental and biological ones separately. The additional columns show the proportion of possible province pairs (with respect to the total number of combinations) which fall within the following separation criteria of R values: >0.75 totally separate; 0.75–0.5 weak overlap; 0.5–0.25 overlap but some separation; <0.25 no separation.

The difference between the sampling approaches is mostly found in the absolute values, but the relative differences between the set of variables are preserved.

The global R value is generally larger for the ENV variables than for the BIO, which implies that the provinces can be more easily distinguished in terms of their environmental features. It is interesting to note that the fraction of provinces which cannot be statistically separated according to the BIO variables is zero with the random sampling, yet it is the highest (0.04) with the SAMP1 procedure. There is thus a slight dependency on the choice of the sampling scheme although there is little effect on the global R value when all the variables are considered.

Overall, 80% of the analysed province pairs were statistically separable ($P<0.05$). We have also listed in

Table 2 the provinces that are statistically not separable (about 3% for all the variables in SAMP1). We focus here on adjacent regions because it is likely that distant regions belonging to different oceans can be characterised by statistically similar features. These regions are therefore "geographically different" but "biogeographically similar". For instance, provinces 56 and 60 in the northern Pacific (see Figure 1) are not separable and adjacent. This indicates that the boundary between 56 and 60 is arbitrarily imposed and the model cannot reproduce the features that led to the a priori classification by Longhurst. On the other hand, provinces 10 and 31 are also both indistinguishable from the northern Pacific subtropical gyre (60), but they are located in geographically distant regions, and each province is separable from the other ones in the same basin.

3.4 Theoretical validity

The previous analyses have shown the existence of distinct regions which have been selected on the basis of a priori knowledge of the physical and biogeochemical features. In this section we will further investigate whether the model shows a direct correlation between the physical environment and the biology, underlining the process dynamics expressed by the model. This effort is defined theoretical or conceptual validity in qualitative research and social sciences, and it deals with the relationships thought to exist between the defined variables of a model (Maxwell, 2002). When comparing with real data, a model has theoretical validity if its underlying theoretical constructs provide a better predictive indicator than does a linear model, (Carley, 1996).

We first focused on the relationship between model variables in the various provinces. To extract such information from the model dataset we compared all the MDS ordinations for each variable (means and standard deviations, cfr. Sec. 2.5) over a given set of provinces and check for the similarity between the different combinations of variables. A second-stage MDS analysis (Clarke and Gorley, 2006) is a helpful tool to highlight the correlations among pairs

of many resemblance matrices. This analysis produces a further resemblance matrix where each element is the Spearman rank correlation coefficient between each pair of matrices.

Since the Longhurst's province have a primary partition in biomes (Coastal, Polar, Westerlies and Trades; Longhurst, 1998) distinguished on the basis of large-scale oceanographic drivers, we did the analysis taking into account this grouping factor and ultimately comparing with the result from all the provinces.

Figure 7 illustrates the MDS results for all the provinces, and for three out of four major biomes (Polar, Westerlies and Trades). The results of a hierarchical cluster analysis are overlaid highlighting the clusters with $\rho>0.3$. The most striking feature which is common to all the figures is the lack of correlation between SST and phytoplankton at the annual scale. This is also true for all the other physical variables in general, although MLD is close to the smaller phytoplankton (P2 and P3) particularly in the polar biome (this occurs for TCD as well). Physical variables correlate better with each other, particularly SST and surface irradiance (SWR). The pattern identified by the MDS shows a cluster around diatoms (P1) comprising all the nutrients (N), bacteria and larger zooplankton. This pattern is typical of seasonally mixed waters, generally dominated by the herbivorous food-web structure during spring (Legendre and Rassoulzadegan, 1995). Indeed, we find the same pattern in the Westerlies biome (Figure 7b), which is defined according to these characteristics (Longhurst, 1998).

In the Westerlies, as in the MDS of all the provinces, the smaller phytoplankton groups are closer to the MLD which may be interpreted as a correlation with stratified conditions. Interestingly, nutrient concentrations are not related to the physical environment which implies that the relationship between phytoplankton and residual nutrient concentrations is not evident at the annual scale in the model.

Iron and salinity are distant from all the other variables and with almost no correlation. This is clear for salinity because it does not enter in the biological parameterizations and additionally, it is biased in these particular model results (Bellucci et al., 2007). Fe is a fundamental element regulating primary production in the model (Vichi et al., 2007a), however, its surface monthly average concentration is low in most of the provinces and therefore it is difficult to see a correlation with the other variables at this scale.

In the Trades (Figure 7c) there is a clear switch between diatoms and picophytoplankton, because the latter are highly correlated with nitrate and phosphate ($\rho > 0.8$). P2, P1 and the other components of the microbial loop (bacteria and HNAN) are close and also clustered together with silicate (though correlation is lower, $\rho > 0.3$). The trades biome represents the climax community of the pelagic ecosystem with high trophic complexity (Longhurst, 2007) though low standing stocks and the model captures this by creating a close correlation between the biological variables. All the physical variables are instead clustered separately, as we might expect from a biome with little physical variability.

The polar biome is the most difficult to interpret, and also the MDS stress is higher with respect to the other biomes, which implies a poorer two-dimensional representation. Nutrients are clustered together with the thermocline depth (TCD) and salinity. A characteristic of the polar biome is the low salinity surface layer, which the model relates to the nutrients but not to phytoplankton. The MLD is again an indicator of smaller phytoplankton, though this is only relevant in the regions of the Antarctic frontal zone and in the Arctic province because picophytoplankton in the model is severely limited by temperature (Vichi et al., 2007a). In fact, SWR and SST are related to each other and slightly closer to the smaller phytoplankton. Diatoms are in good rank-correlation with zooplankton, indicating a likely dominance of the trophic control. The relationship between iron (N7) and the microbial loop is difficult to interpret. The MDS pattern is indeed rather peculiar, with small clusters equally distant from

each other and from the centre of the graph. It is likely that given the large model bias in the simulation of the Southern Ocean, we cannot consider this graphical representation as explicative as the others.

3.5 External validation with satellite chlorophyll

This section considers the objective comparison with independent data from the SeaWiFS level 3 mapping. The multivariate dataset consists of the annual mean chlorophyll concentration for each province, the spatial standard deviation of the annual mean and the temporal standard deviation of the monthly data (cfr. Sec. 2.5).

3.5.1 Chlorophyll provinces

A possible objective test of relations between data and model is the computation of the Spearman rank correlation coefficient (ρ) and the RELATE test statistics (Clarke and Gorley, 2006). Data have been first log-transformed and normalised, then the resemblance matrices have been computed as Euclidean distances between the variable values of each province. The value of ρ is between -1 and +1 while 0 means there is no match between the similarity matrices. The null hypothesis is no absolute relationship between the two data sets. The actual ρ is compared with a frequency table of ρ values obtained from random permutations of the values in the resemblance matrices. One million permutations is used as default since the number of samples and variables is rather small.

The test applied to all the provinces gives a ρ-value of 0.183 ($p>4\%$) which changes to 0.323 ($p>0.2\%$) if the coastal provinces 11 and 12 are removed. This implies that the model and data are only weakly related yet the matching pattern is statistically significant at least in the open ocean areas. The value of ρ can thus be used as an overall indicator of the model versus data matching and taken as benchmark for further validation exercise with respect to model improvements.

It is also interesting to verify whether chlorophyll provinces are statistically separated both in the model and in the data. The ANOSIM test was performed on the randomly sampled data from the SeaWiFS and model data. Global R statistics are both below 0.25, which implies that the provinces cannot be statistically separated neither in the data nor in the model. On the contrary, Hardman-Mountford et al. (accepted) did find significant dissimilarity between SeaWiFS data samples extracted from different putative biomes in the Pacific Ocean. A possible interpretation of the small separation found in our data analysis might be related to the arbitrary choice of the province boundaries, which is not necessarily the same of the provinces derivable from SeaWiFS (Hardman-Mountford et al., 2007, accepted). It is likely that SeaWiFS province features are smeared out when there is a mismatch between them and the boundary of predefined Longhurst provinces on the model grid (Figure 1).

3.5.2 PCA of Longhurst provinces

Figure 8 presents the results of a PCA performed on the log-transformed and normalised model and satellite chlorophyll datasets, where the coastal provinces have been neglected as done in the RELATE test above. This is a correlation-based PCA, because the log transformation reduces any weighting towards high chlorophyll provinces and the normalisation equally weights the means and the second order moments. Our aim here is to investigate whether chlorophyll statistical properties derived from the model and the satellite correlate in a similar manner among the provinces. Given the high overlap between provinces shown in the section above, we do not focus on the specific location of each province in the PCA space but we are more interested in the qualitative (eigenvector pattern) and quantitative (eigenvalues) assessment.

The figure lists the percentage of variance explained by the first three components for each dataset. The plots show the magnitude and sign of each variable's contribution to the first two PCs and the scores of each province. A sign convention has been imposed in the layout of

the eigenvalues to force the elements with the largest magnitude to be in the positive quadrant. The first PC explains a large portion of the variance in both datasets, although the model is characterised by much lower contributions of the remainder components. It is interesting to note that if the Southern Ocean and the northern Indian provinces (which are characterised by the largest biases) are removed from the analysis, the eigenvalues tend to match and also the percentage of variance explained by each component.

We observe that both PELAGOS and SeaWiFS data have the spatial standard deviation in the upper right quadrant together with the mean, and the seasonal variability in the lower right quadrant. We can argue that the dominant mode (PC1) of both datasets is equally described by the contribution of the spatial variability and mean values, although the model is less capable to represent the spatial variability inside each province (i.e., PC2 which is related to spatial standard deviation explains much less variance in the model results).

3.5.3 PCA of seasonal maps

Figure 9 shows the eigenvalues and percentage of variance contributions of each principal component (PC) from spatial mode PCA of mean monthly chlorophyll maps (1997-2001 average) from PELAGOS and SeaWiFS. The first PC from SeaWiFS overwhelmingly dominates the variance (80.8%) whereas PELAGOS requires the first two PCs to explain this level of variance (PC1=65.8%, PC2=16.6%).

Figure 10 shows the eigenvectors, or loadings, for the first 3 PCs for both SeaWiFS and PELAGOS. These show the correlation of each time step to the PC image (score). The eigenvector plots show that the temporal amplitude of the pattern in PC1 exhibits very little variability, with the pattern being strongly present throughout the year. Higher order PCs show temporal amplitudes related to different modes of seasonal variability, but these modes each represent only a small part of the total variance. For SeaWiFS two distinct annular modes are represented by the eigenvectors for PC2 and PC3. For PELAGOS, a somewhat

smoothed annular mode is represented by the eigenvector for PC2, qualitatively comparable to the eigenvector for PC2 of SeaWiFS data, however, the eigenvector for PC3 in PELAGOS is clearly not representative of that in SeaWiFS.

Given the low eigenvalues of all but the first PC for both data sets, only PC images for the first PC are shown in Figure 11 and this is the only PC further considered here.

Within the PC1 images, distinct large-scale ocean regions are distinguishable, differentiated by distinct gradients. For SeaWiFS, high chlorophyll patterns are seen in coastal and shelf regions (including coastal upwellings and river mouths; red to orange colours). Oceanic upwellings, frontal regions and extended river plumes with intermediate chlorophyll patterns are shown in yellow to green colours. Lower chlorophyll patterns in the central ocean gyres range from cyan through blue to magenta. A fuller explanation of these patterns is given by Hardman-Mountford et al. (accepted).

From these patterns, there is clear alignment with Longhurst's biomes in most areas, but with the equatorial region more clearly delineated than in Longhurst (1998). On a broad scale, PELAGOS simulates these major biomes (gyres, mid-latitude westerly regions, equatorial zones). However, several differences are notable between the patterns in SeaWiFS and PELAGOS: (1) PELAGOS is underestimating the chlorophyll concentration in coastal margins and overestimating in the Southern Ocean; (2) central ocean gyres are clearly visible in PELAGOS for the Atlantic and Pacific Oceans, but their chlorophyll concentrations are generally overestimated, especially in the South Atlantic, but with some areas of underestimation in the North Pacific; (3) the chlorophyll structure of the Indian Ocean bears no resemblance to SeaWiFS; (4) the region of equatorial upwelling and current systems overestimates chlorophyll in the Pacific Ocean and underestimates for the Atlantic Ocean.

4 Discussion

Our study emphasizes the use of multivariate statistical techniques as tools for the skill assessment of global ocean biogeochemical models. Specifically, we have analysed the results of one of the most comprehensive biogeochemistry models to demonstrate that such techniques are helpful to elucidate the mechanisms of the model and to assist the comparison with various sources of data. MDS highlights qualitative distances between samples in a reduced dimensional space, without any implied suggestion of what factor is causing the observed separation. MDS is thus used here as an investigation tool to objectively depict and analyse model results.

The results have elucidated several aspects of model behaviour. Primarily, the model does have emergent biogeographic provinces, which are obtained as the combined effect of physical constraints and biological response. We recognize that the predefined set of provinces is arbitrary, as well as the boundaries between them. However, the ANOSIM test demonstrates that the separation between provinces, based on the chosen set of variables, is statistically significant, implying that Longhurst's provinces are present in the model and are more significantly separated in the environmental data than in the biological data. This result is a confirmation that the use of adequate physical GCM simulations is an important prerequisite for the identification of biogeographic provinces through models, e.g. Gregr and Bodtker (2007).

Further insights can be inferred from this analysis. The MDS representation of the biological variables is different from the one obtained by the environmental variables. We have shown with the aid of a second stage MDS (Sec. 3.4) that the correlation between the major environmental variables and biology (particularly with SST) is not as large as expected. Therefore the definitions of biomes in the model are not easily derived from direct (rank) correlations between physical conditions and biological response. This indicates that the

biogeochemical model is not acting as a simple linear interpolator of the physical dynamics, though it does not necessarily mean that it is capturing the underlying dominant drivers of the real ocean biogeochemistry.

We must bear in mind that the bio-physical provinces obtained from this kind of model may not be the same as classical ecological province definitions. Provinces are generally defined either by environmental characteristics but also by species composition or by a combination of several ecological factors (Longhurst, 2007). A deterministic biogeochemistry model operates, by definition, at the level of ecosystem function. Functional ecology doesn't necessarily separate out in the same way as environmental or species level provinces. On the other hand, if provinces are representative of macro-scale ocean ecosystems, then the physical, ecological and biogeochemical properties should be aligned and functional representations should be able to simulate these ecosystems over realistic temporal and spatial scales.

The results of Sec. 3.4 show that all nutrients tend to be rank-correlated to primary producers without an indication of a specific limitation. On the one hand this can be interpreted as an over-parameterization of the number of important nutrients, but also as an aspect of co-limitation (the functional response is independent of one single nutrient because it is the bulk limitation effect which regulates the behaviour). Iron on the other hand behaves quite differently with respect to the other nutrients, though it is known that iron limits production in the model by definition. If Fe-limitation is removed, the overestimation of diatom production is remarkable (Vichi et al, 2007b). This implies that the seasonal variability of iron residual concentration in the water cannot be taken as a measure of potential production. The mismatch between classical functional relationships between the variables needs further clarification. Our methodology can be helpful in assessing the

theoretical and process validity of different configurations of the model, for example by reducing the number of nutrients or the number of biological functional groups.

To understand ocean ecosystem functioning and interactions at the sub-seasonal scale, spatial resolution of mesoscale features is probably required, as well as finer resolution of the inter- and intra-specific variability within the simulated populations of PFTs. However, if the key properties of the province are effectively captured and the model is statistically capable of distinguishing the major regions of the ocean, we might argue that these kind of results are appropriate for seasonal and long term studies of climate variability.

As a proof of concept, we have limited our analysis to the comparison with SeaWiFS data which is presented in Sec. 3.5. PCA provides a quantitative comparison of the relative contribution of different PCs to the total variance. The associated temporal and spatial patterns aid interpretation but the eigenvalues measure how well the model is capturing dominant modes of variability compared to observations. The first one-to-one comparison indicated that both the model and SeaWIFS data are dominated by quasi-steady-state spatial structures, representative of biomes and provinces. The model shows stronger seasonal variability than the SeaWiFS data. Homogeneous regions where the seasonal variability (or the lack of it) is dominant are likely to be better captured by the model. The model thus demonstrates objective skills because it captures the dominant mode despite the macroscopic mismatch in certain regions (e.g. Indian and Southern Ocean).

The use of the RELATE test is an overall measure of model goodness-of-fit, which is still rather low (0.323), provided that the coastal provinces are removed from the analysis. On the other hand, it needs to be considered that the separation between the subjectively-determined Longhurst provinces is fixed *a priori* and does not necessarily coincide with the provinces that can be derived from the non-interpolated SeaWiFS data (Hardman-Mountford

et al., 2007, accepted). This explains why the ANOSIM test found little separation between the Longhurst provinces identified in terms of chlorophyll values.

5 Conclusions and future work

Our approach applies the concept of provinces as a diagnostic tool for the analysis and validation of global marine biogeochemistry models. It is suggested as a method of overcoming the limitations to model verification imposed by data scarcity and the general under-sampling of relevant ocean biogeochemical properties.

The MDS has shown that intuitive province,s derived by *a priori* considerations, are coherently distinguished in the model. Longhurst biomes and provinces do exist in the model results though it is not yet proven whether they are characterised by the same properties as in the real ocean. A first comparison with satellite-derived chlorophyll emphasized a mismatch between the provinces definition when applied to SeaWiFS data and to model results, but with some agreement at the biome level. The application of MDS, together with ANOSIM, provides a powerful tool for the interpretation of model results. We recommend their use in the validation process of OBGCM and especially in objective comparisons with data. This implies the use of multivariate datasets with a global ocean coverage, which are only partly available. Nutrient maps have been objectively derived from the World Ocean Dataset (Conckright et al., 2002) and can be used together with SeaWiFS data to build MDS representations and compare them directly with the corresponding MDS from model output.

The first-order analysis has to be forcibly based on bulk properties, because these are currently the only data with sufficient spatial and temporal coverage. The new available global products of PFT distributions (e.g. Sathyendranath et al., 2004; Alvain et al., 2005; Aiken et al., 2007; Hirata et al., accepted) will provide a substantial aid for the objective validation of the PFT model results. Additionally, the strength of our approach is that once the province is defined as statistically separate from the others and characterised by consistent

and coherent properties, other more ecologically relevant information can be extracted from the model results and compared with local datasets which are usually more reliable (e.g. Bouman et al., 2006; Olguìn et al., 2006). This might help to overcome the mismatch between station data and large-scale model results without the need to extrapolate sparse, low-frequency measurements.

The further step in our approach is to derive the provinces directly from the model results. A similar approach was done by Sarmiento et al. (2004) defining the regions by means of an empirically-derived, linear combination of physical properties such as SST, mixed layer depth, etc. Gregr and Bodtker (2007) refined this method by substituting the interpolation with a multivariate adaptive classification algorithm. A likely alternative would be to use unsupervised neural networks such as Self-Organising Maps (Kohonen, 2001) in a similar way to Allen et al. (2007). Grid points with similar bulk properties are likely to be grouped together, defining the boundaries in a more coherent way which would thus be dependent on the model dynamics.

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Tables

Table 1 Surface ocean with area-weighted sampling (SAMP1) and random sampling with 20% of total surface grid points (SAMP2). The third column reports the fraction of pairs with significant relationship ($P<0.05$) and the remainders are the fractions of significant pairs which fall within the given similarity limits.

SAMP1	**Global R**	**P<0.05**	**>0.75**	**0.50-0.75**	**0.25-0.50**	**<0.25**
ALL	0.56	0.84	0.52	0.16	0.13	0.03
ENV	0.61	0.87	0.54	0.18	0.12	0.02
BIO	0.44	0.70	0.38	0.17	0.11	0.04
SAMP2	**Global R**	**P<0.05**	**>0.75**	**0.50-0.75**	**0.25-0.50**	**<0.25**
ALL	0.60	0.95	0.47	0.33	0.13	0.02
ENV	0.62	0.95	0.48	0.30	0.15	0.01
BIO	0.52	0.84	0.39	0.24	0.18	0.0

Table 2 Province pairs which are statistically not separable according to the ANOSIM test (R<0.25) on the environmental and biological variables. Only the pairs with P<0.05 have been considered.

ANOSIM SAMP1: P<0.05, R<0.25			
6 (NASW),	31 (ISSG)	10 (SATL),	60 (NPTG)
6 (NASW),	59 (SPSG)	31 (ISSG),	56 (NPSW)
7 (NATR),	32 (EAFR)	31 (ISSG),	60 (NPTG)
10 (SATL),	31 (ISSG)	54 (NPPF),	59 (SPSG)
10 (SATL),	56 (NPSW)	56 (NPSW),	60 (NPTG)

Figure captions

Figure 1 Location, names and numbering of selected Longhurst's provinces on the model grid.

Figure 2 Visual comparison of the simulated chlorophyll annual mean with SeaWiFS chlorophyll (1997-2003) interpolated onto the model grid.

Figure 3 Visual comparison of the simulated and observed seasonal cycle of chlorophyll in the North Atlantic Drift Province and Pacific Equatorial Divergence. Satellite data from SeaWiFS and CZCS. Bar plots provide an overview of the most abundant phytoplankton group for each month.

Figure 4 MDS ordination of the full set of variables (environmental and biological). The contours represent the clusters at given distances. The symbols are the results of the SIMPROF test. Similar symbols identify provinces which cannot be significantly separated in further clusters.

Figure 5 MDS ordination for the environmental variables.

Figure 6 MDS ordination for the biological variables.

Figure 7 Second-stage MDS ordinations of model variable data. The contour indicates the 0.3 rank-correlation level identified through a hierarchical cluster analysis. (a) All provinces; (b) provinces belonging to the westerlies biome; (c) trades biome; (d) polar biome.

Figure 8 PCA of model (modchl) and satellite chlorophyll (satchl) properties (mean, spatial standard deviations = stdS and temporal standard deviation = stdT) in all provinces (excluding coastal provinces).

Figure 9 Eigenvalues and % of the total variance explained by each eigenvalue for spatial PCA of SeaWiFS chlorophyll-a climatology and PELAGOS model climatology.

Figure 10 Eigenvector (loading) plots for the first three principal components for a) PELAGOS chlorophyll-a climatology, b) SeaWiFS chlorophyll-a climatology.

Figure 11 First principal component from monthly climatology of PELAGOS chlorophyll (panel a, explained variance = 66%) and SeaWiFS chlorophyll (panel b, explained variance = 81%). The colour scale is linear with arbitrary units after normalisation and PCA transformation.

Figure 01

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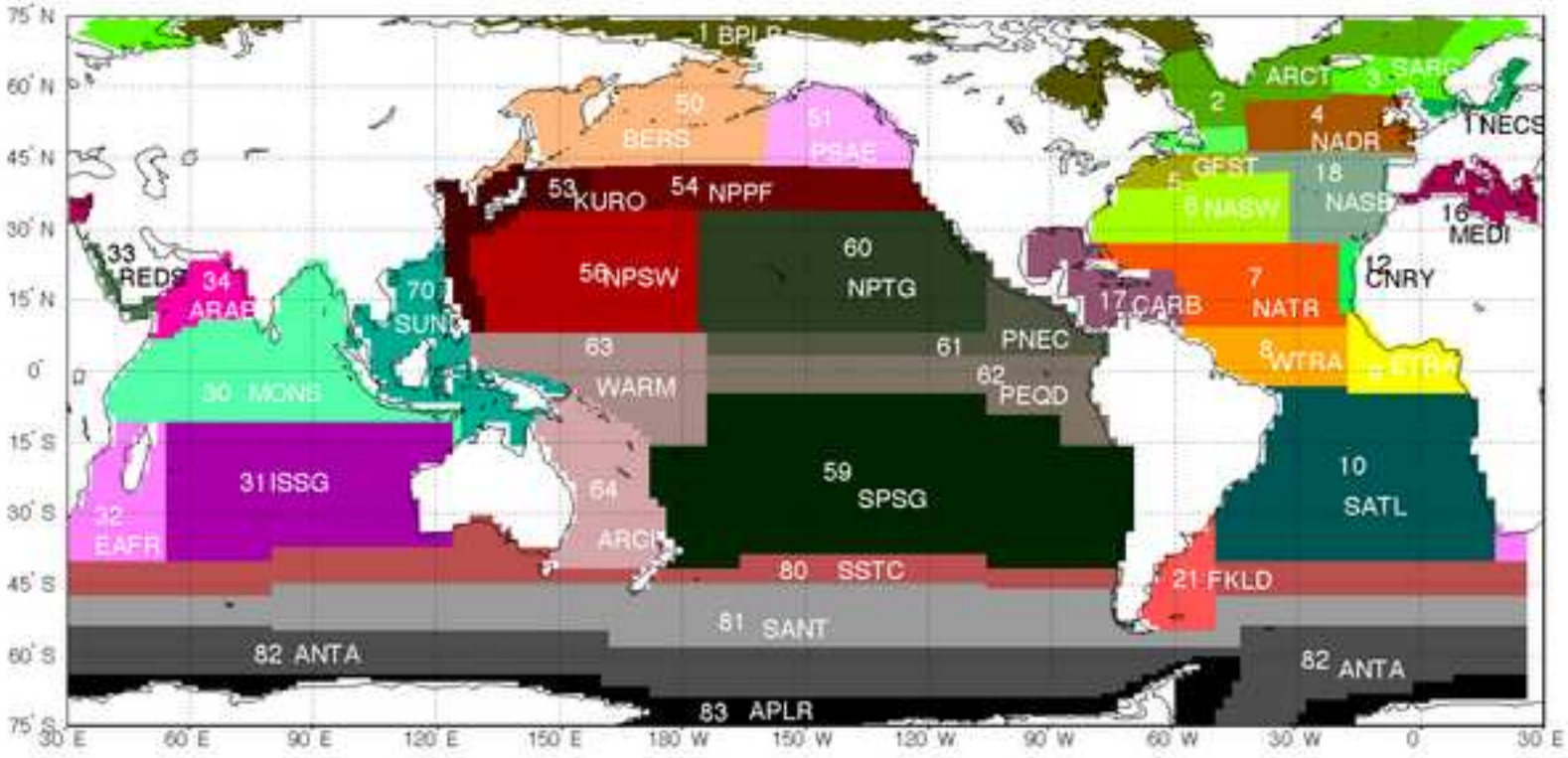

Figure 02a

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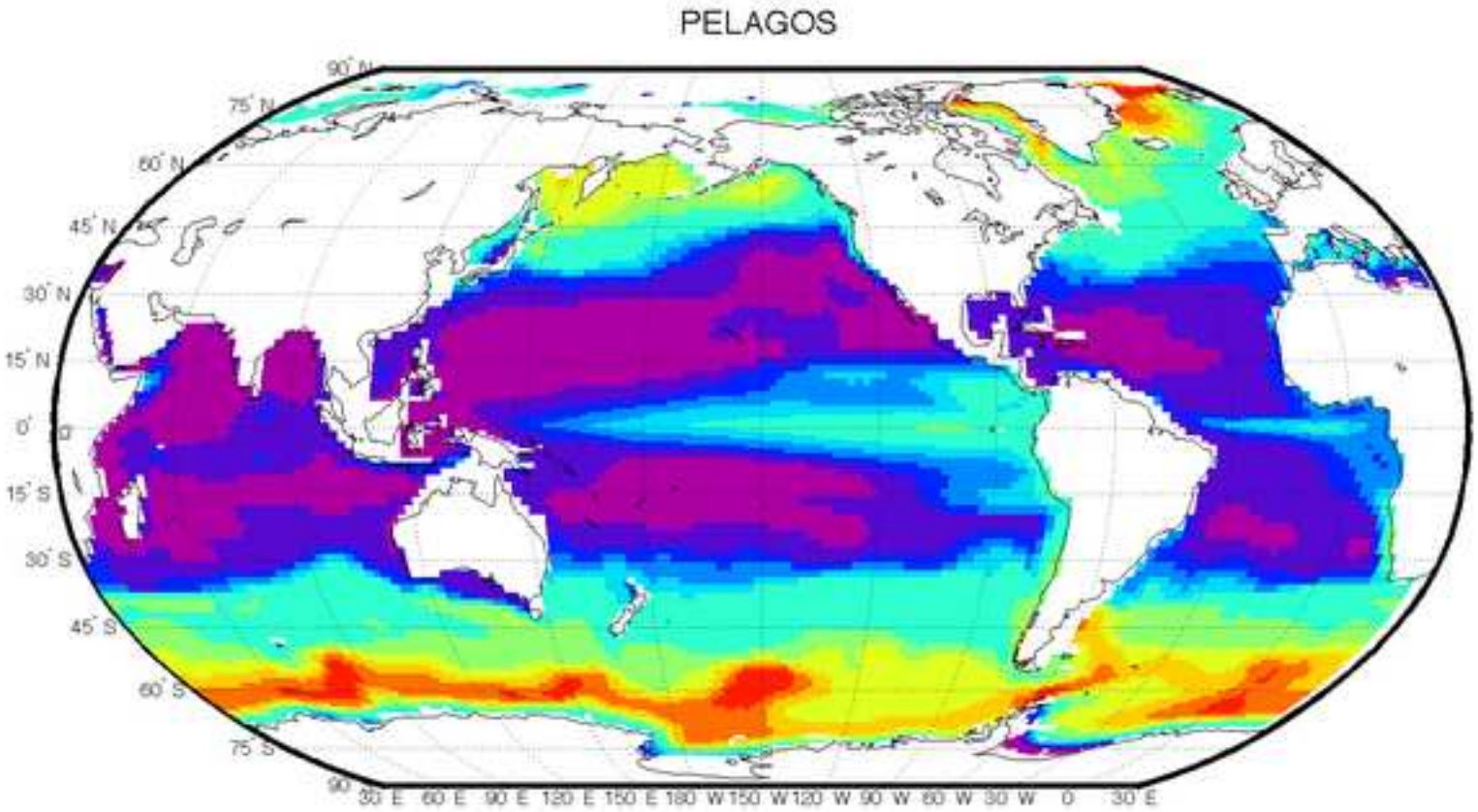

Figure 02b

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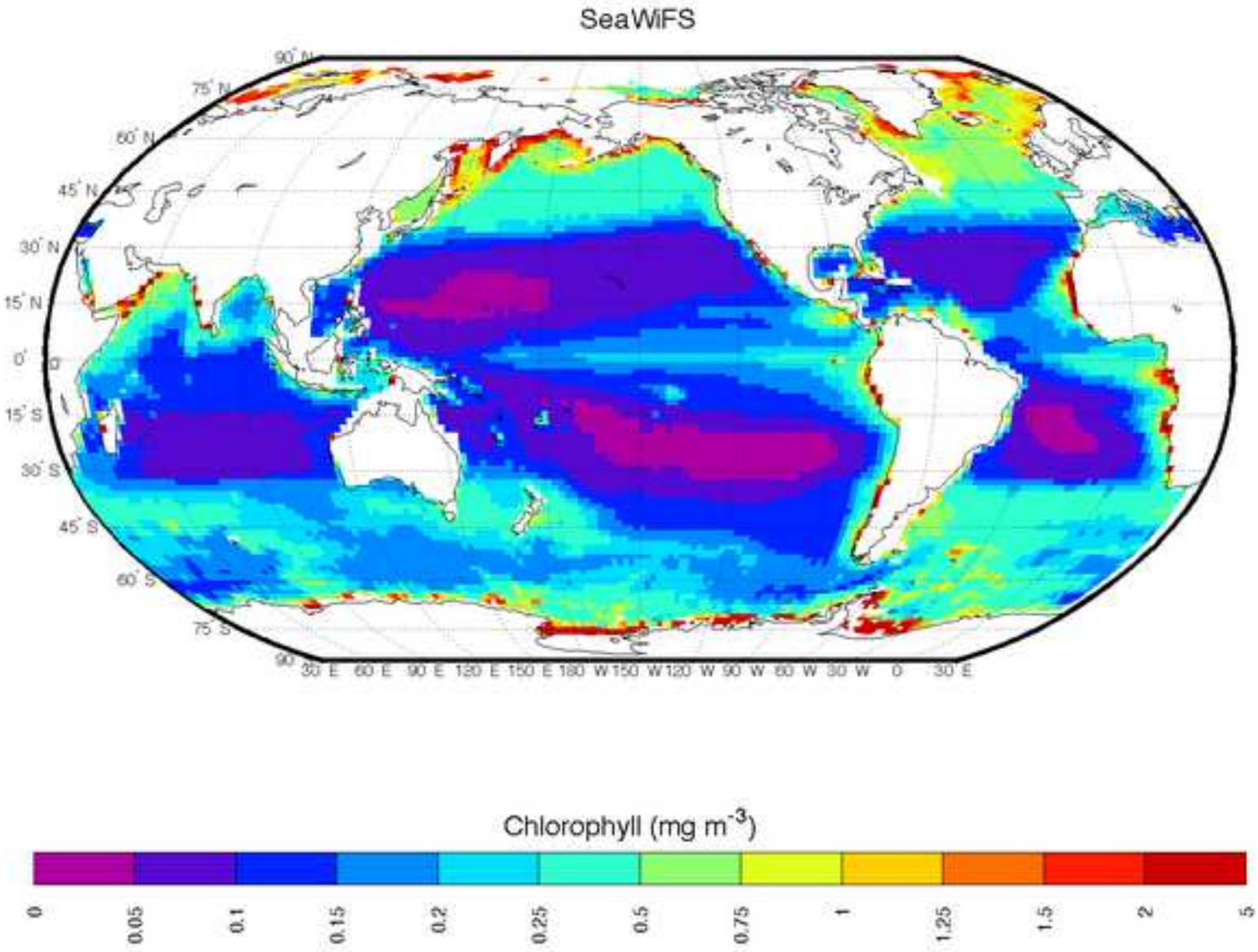

Figure 03

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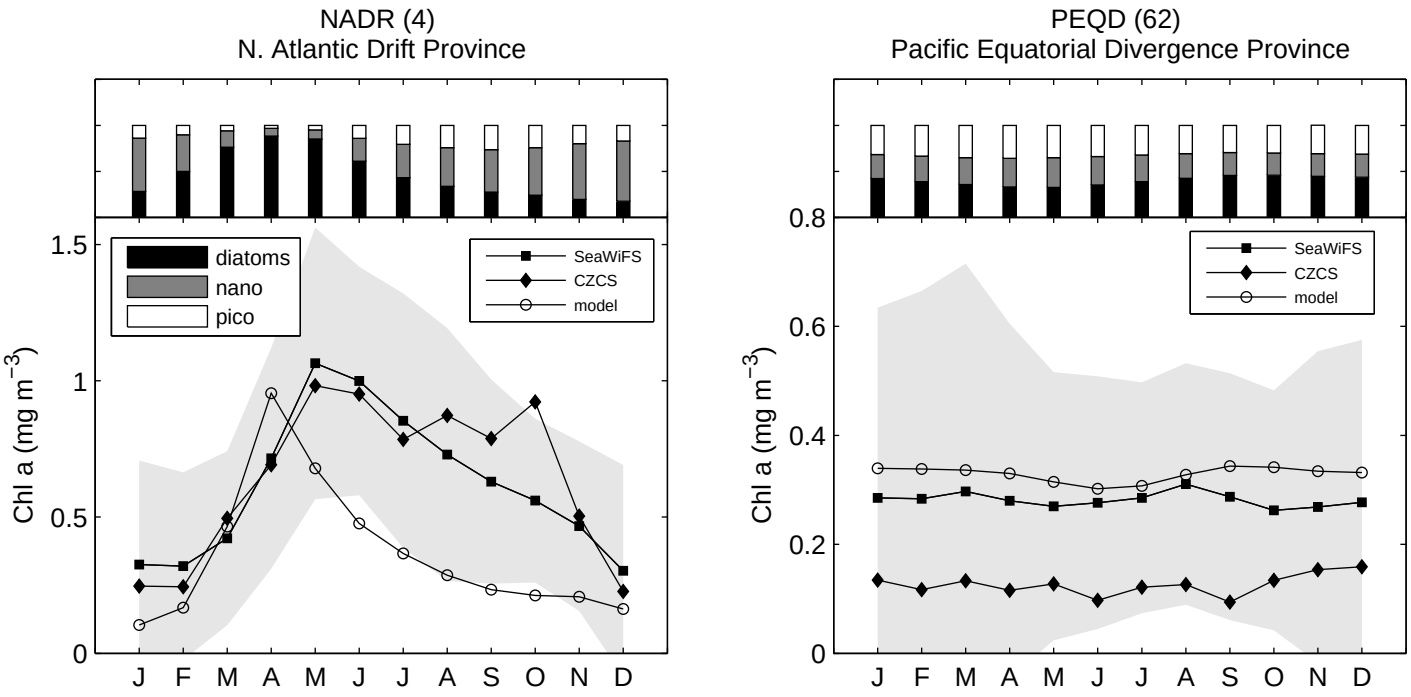

Figure 04

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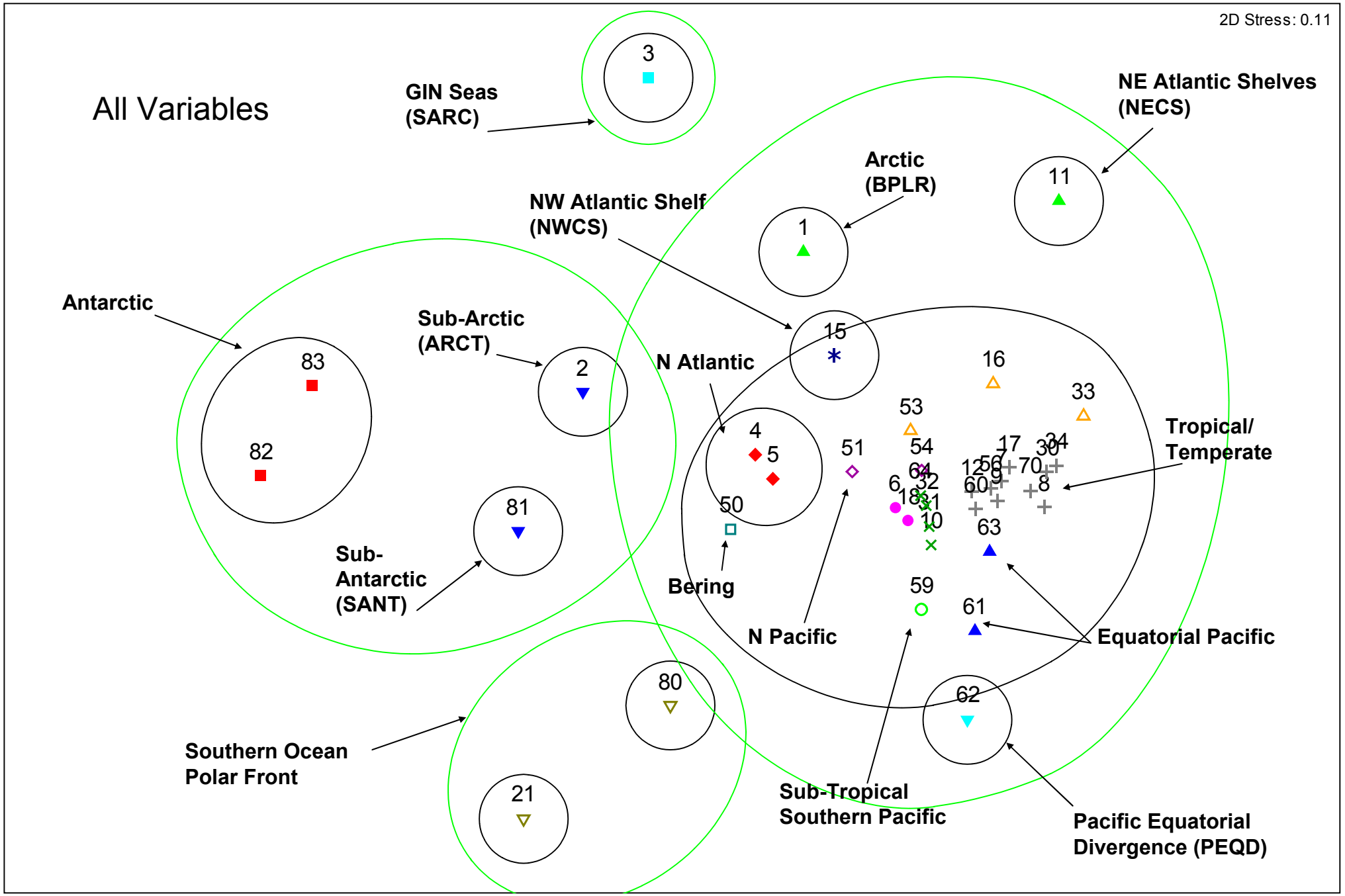

Figure 05

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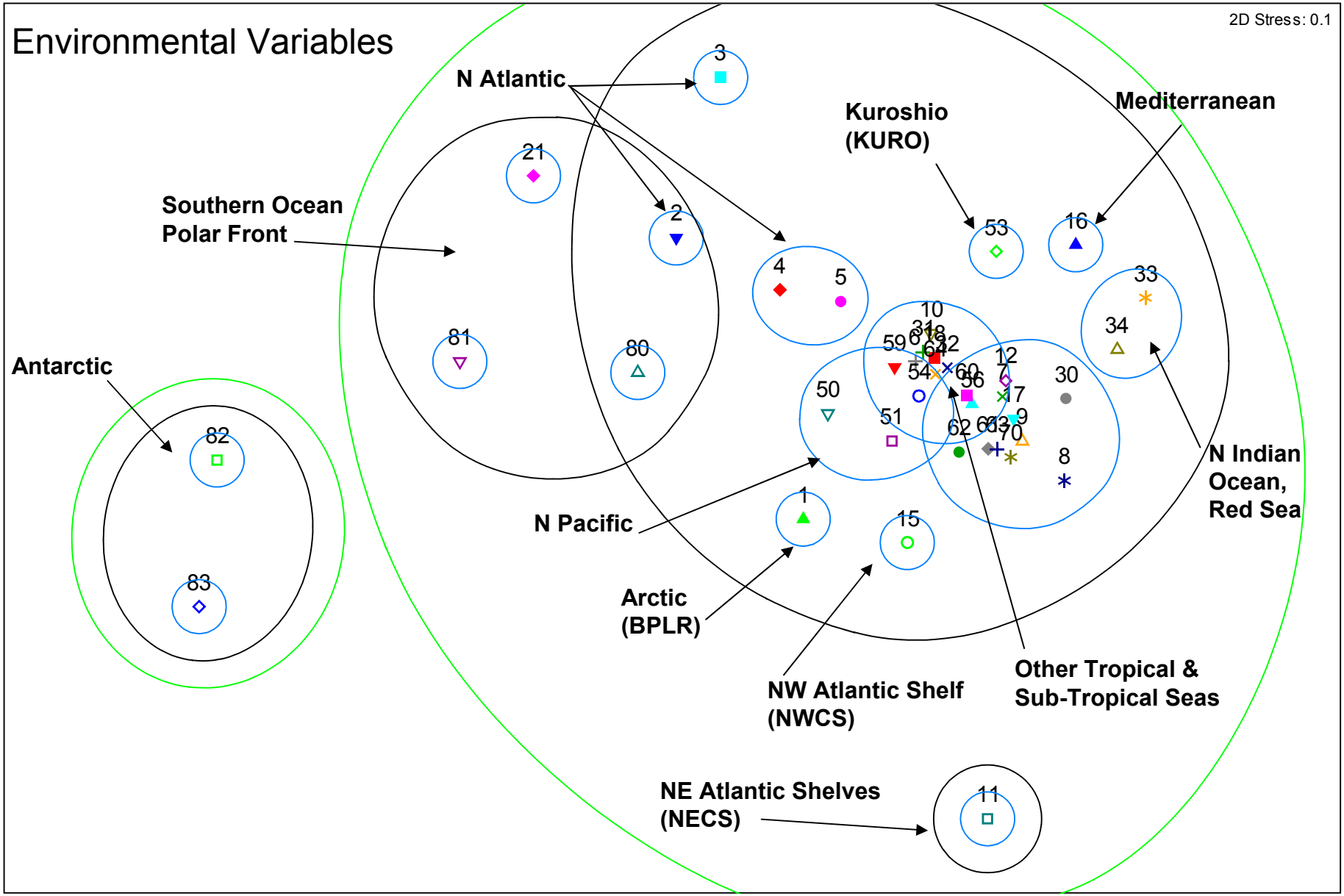

Figure 06

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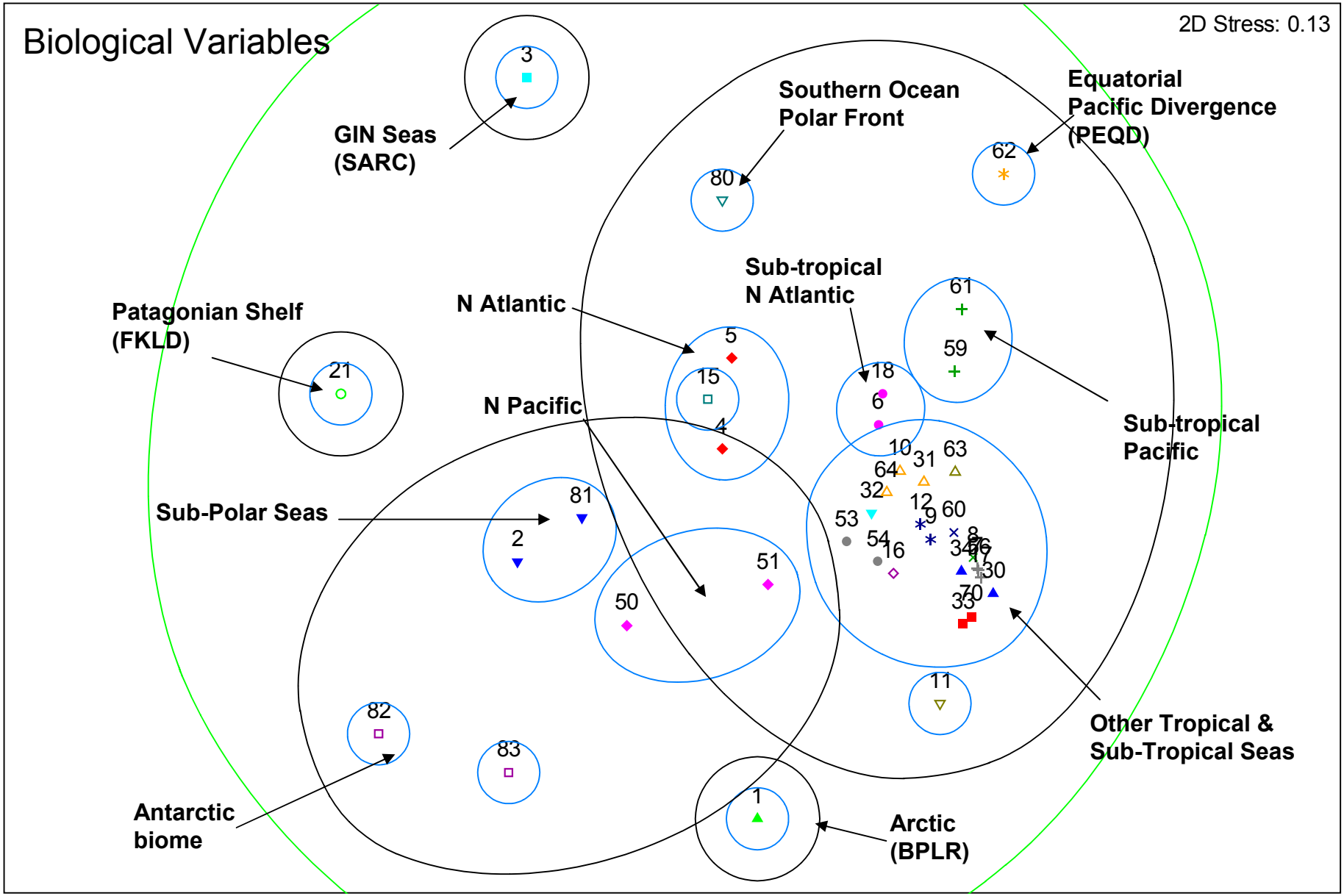

Figure 07

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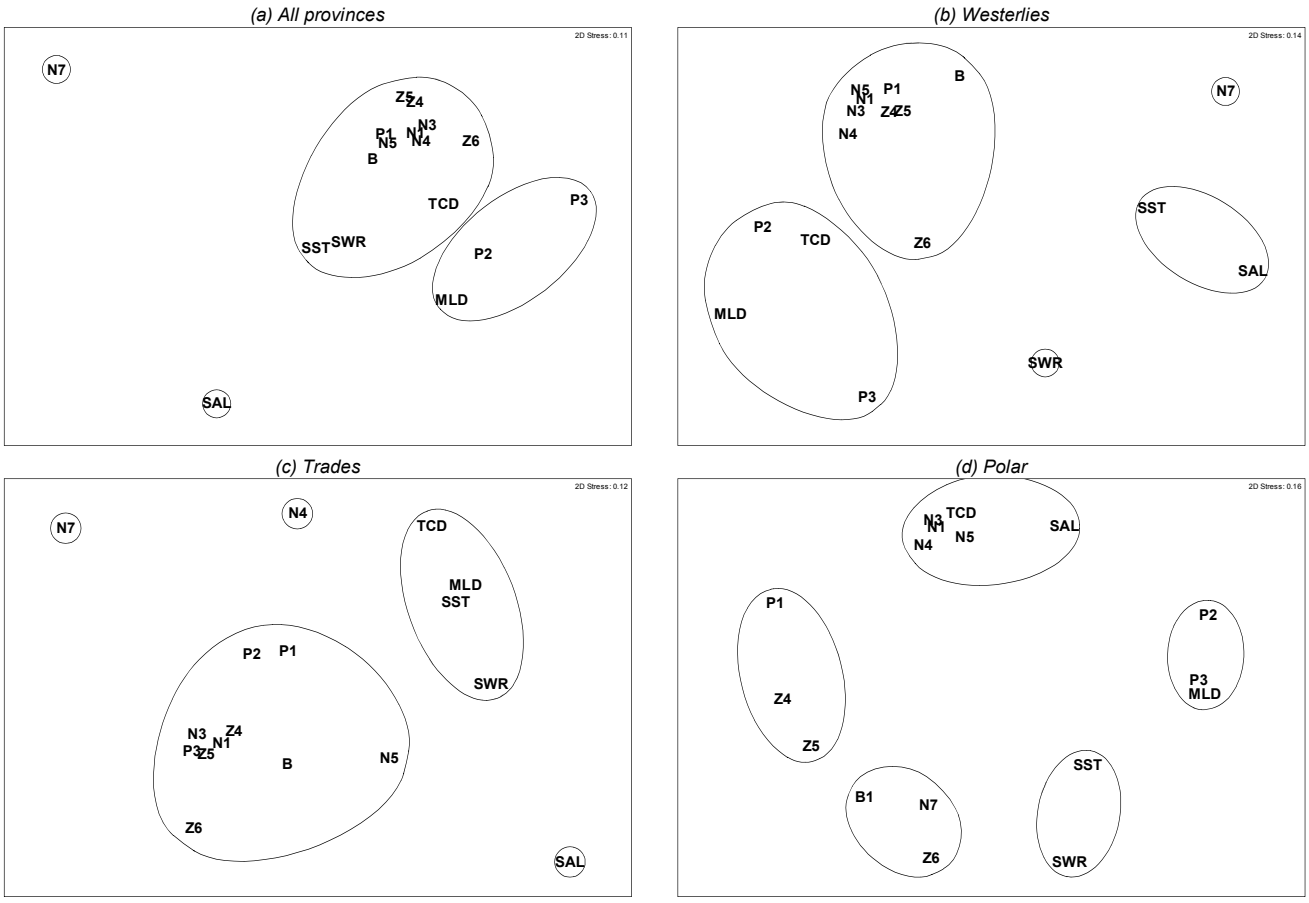

Figure 08

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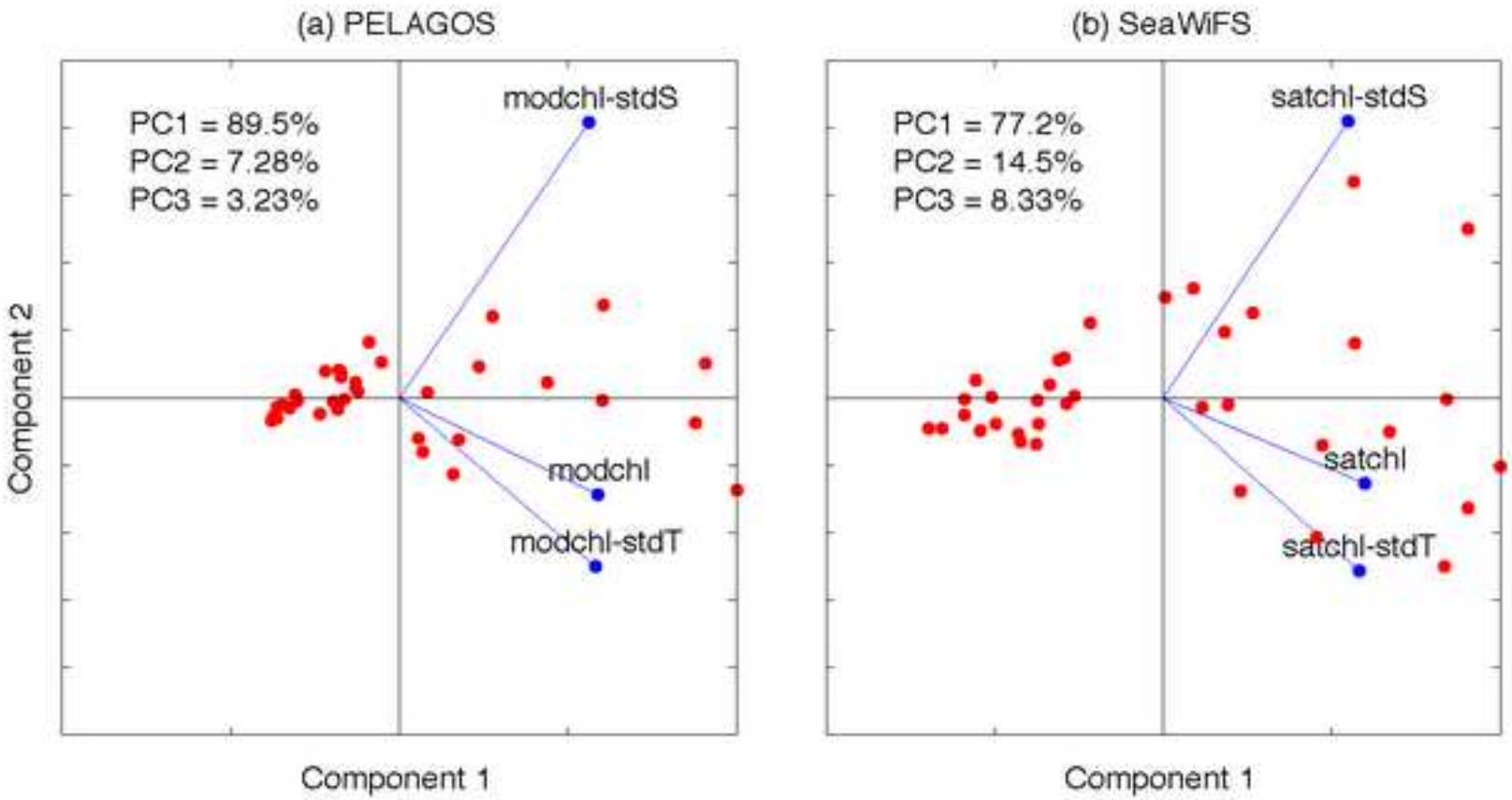

Figure 09

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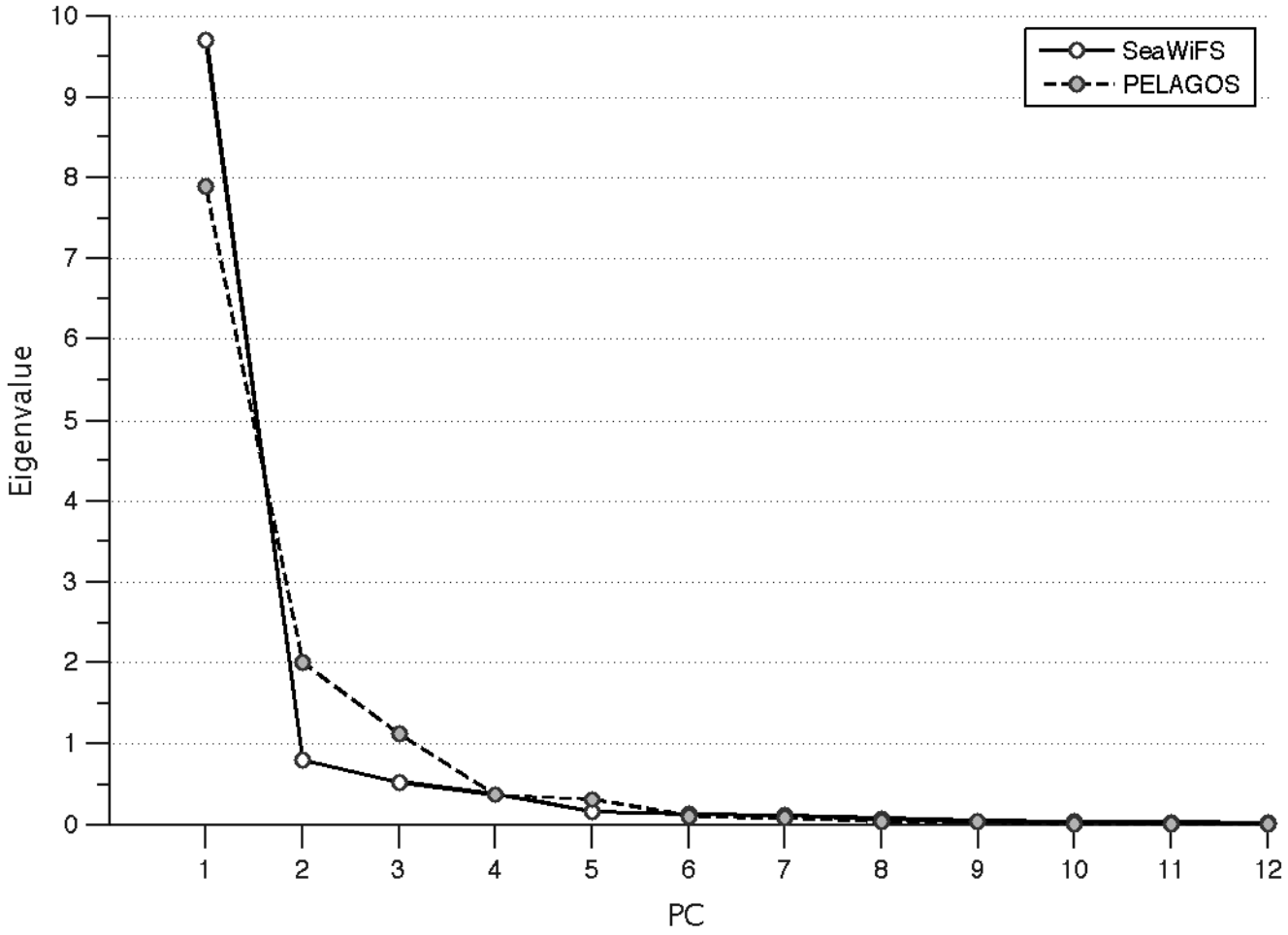

Figure 10

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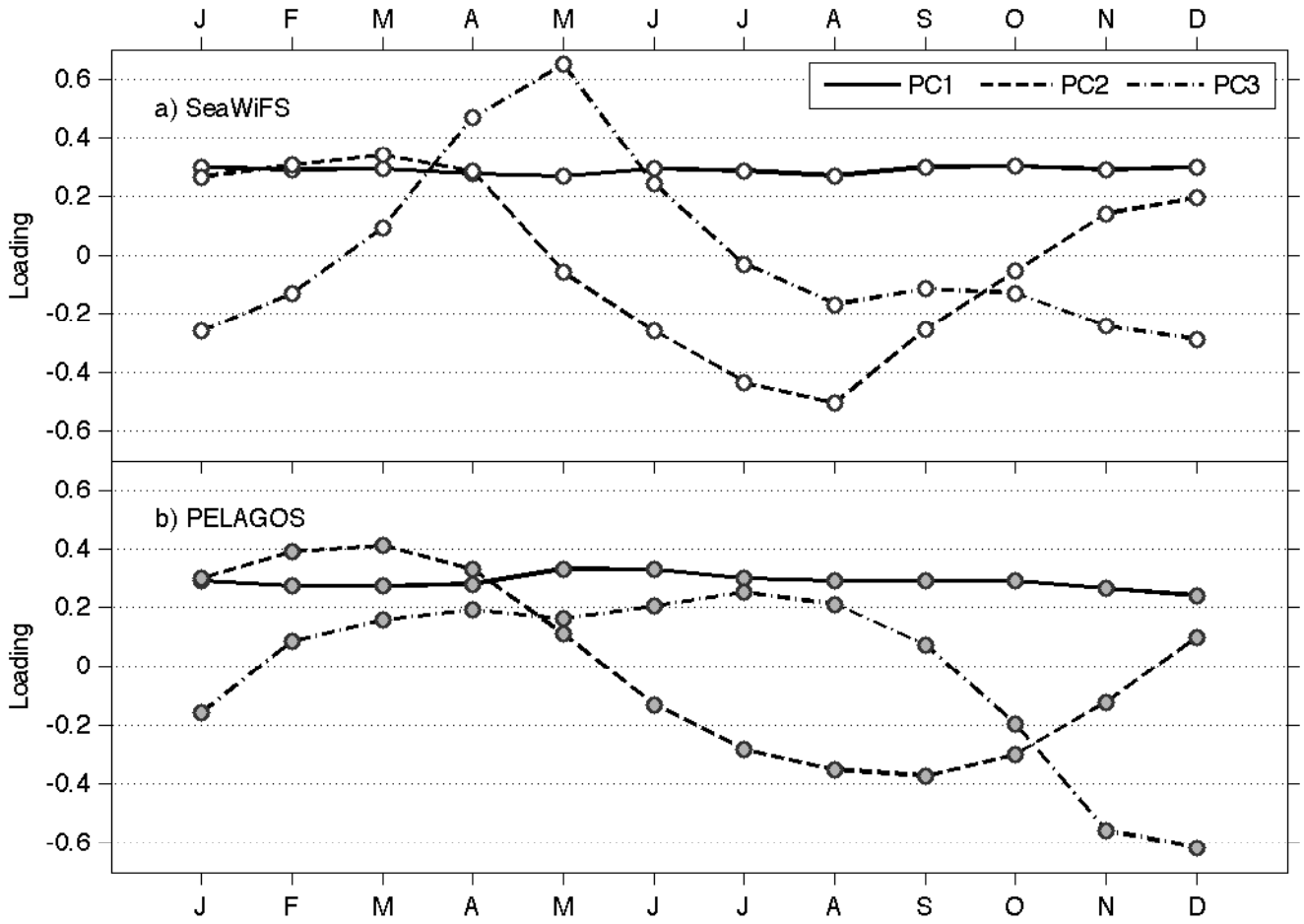

Figure 11
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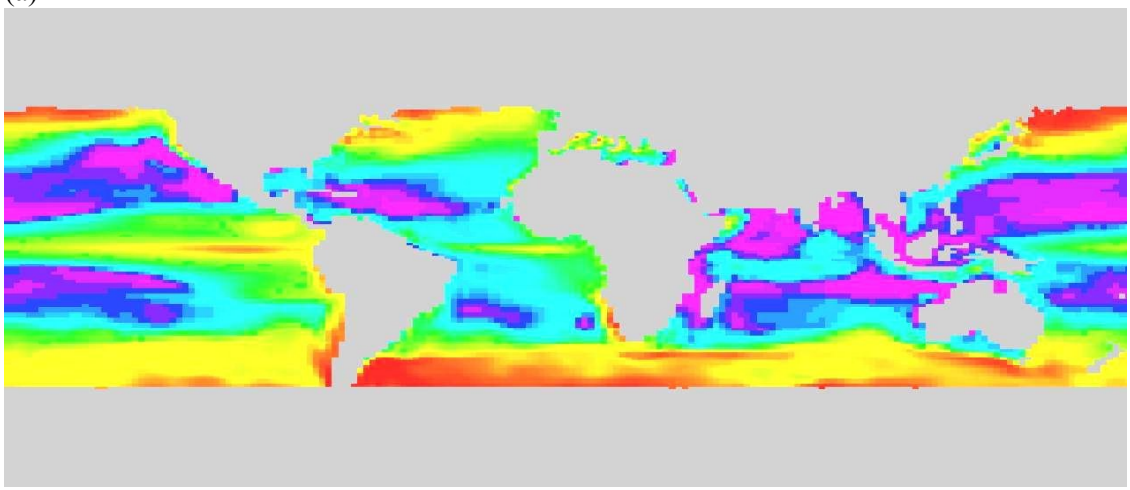
(a)



(b)